



Super Class of Implicit Extended Backward Differentiation Formulae for the Numerical Integration of Stiff Initial Value Problems

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Abstract


An implicit Superclass of non-block Extended Backward Differentiation Formulae (SEBDF) for the numerical integration of first-order stiff system of Ordinary Differential Equations (ODEs) in Initial Value Problems (IVPs) with optimal stability properties is presented. The stability and convergence properties of the SEBDF schemes show that the methods are consistent, zero stable and convergent. The plotted Region of Absolute Stability (RAS) of the methods using boundary locus shows that the methods are A-stable of order up to order 5 and $A(\alpha)$ -stable of order up to 9. The algorithm is described whereby the required approximate solution is predicted using classical explicit Euler's method and conventional Backward Differentiation Formula (BDF) schemes of order k and then corrected using a Super class of Extended Backward Differentiation Formula (SEBDF) schemes of higher orders $k+1$. The SEBDF schemes are implemented using a Modified Newton iteration algorithm iterated to convergence in which some selected systems of first-order stiff IVPs are solved, and the numerical results obtained for the proposed methods are often better than the existing BDF and SBDF methods for solving stiff IVPs.

Keywords: Stiff, Backward differentiation formula, Extended backward differentiation formula, A-stability, Convergence, Consistency.

1 | Introduction

In this paper, our focus is on the numerical approximation of the Initial Value Problem (IVP) characterized by the stiffness of the form:

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$$y' = f(x, y), y(x_0) = y_0, a \leq x \leq b. \quad (1)$$

The stiff Ordinary Differential Equations (ODEs) are a class of IVPs in which the dynamics involved exhibit widely varying time scales [1]. Stiffness is a concept that doesn't have a universally accepted definition but is highly significant in the context of numerical solutions for differential equations; its determination depends on factors such as the specific differential equations, the initial conditions, and the chosen time interval for analysis.

Stiff differential equations are distinguished by their requirement for an exceptionally small step size to integrate their solutions precisely. In simpler terms, these equations typically involve at least two time constants, where time serves as the common independent, and these constants exhibit a significant difference in the order of Magnitude [2].

These IVPs involving stiff ODEs are encountered in various fields of science and engineering, including electrical circuits, vibrations of strings, control systems, nuclear decay, reaction kinetics, and aerodynamics [3]. They also have applications in astrochemical kinetics, computational fluid dynamics, and mechatronics and extend to non-industrial domains like biology, weather forecasting and prediction [4].

In recent years, significant attention has been directed towards developing efficient numerical algorithms for numerically integrating stiff systems. Despite various proposed algorithms, the Backward Differentiation Formula (BDF) was introduced in [5], and the BDF scheme is a numerical method used for the integration of ODEs. It results from the modification of the well-known general k-step Linear Multistep Method (LMM) and is particularly designed for stiff ODEs. This BDF algorithm is given by

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k}, \quad (2)$$

The coefficients α_j and β_k are usually determined to ensure basic desirable properties such as order and its Local Truncation Error (LTE), stability, convergence and accuracy. These BDF algorithms are A-stable for orders 1 and 2 and $A(\alpha)$ -stable from order 3 up to order 6 [6]. The extension to non-block fixed point BDF schemes often involves introducing additional parameters in Eq. (2) to improve stability and accuracy, as in [7], and the scheme is represented as

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k (f_{n+k} - \rho f_{n+k-1}), \quad (3)$$

Cash in [8] introduced a set of EBDF schemes designed for the approximate numerical integration of stiff systems involving first-order ODEs. The algorithms involve predicting the required approximate solution using a conventional BDF and subsequently correcting it with a higher-order EBDF scheme. This methodology enables the creation of A-stable schemes of orders up to 4 and $A(\alpha)$ -stable schemes of orders up to 9. The algorithm is given by

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \beta_k f_{n+k} + h \beta_{k+1} f_{n+k+1}. \quad (4)$$

Several decades ago, the algorithms mentioned above stood the test of time, remaining among the most effective general-purpose techniques for the numerical integration of stiff ODEs. The EBDF algorithms prove advantageous, especially when traditional explicit methods become computationally expensive due to the necessity of very small step sizes. These algorithms strike a delicate balance between accuracy and stability, rendering them applicable to a broad spectrum of stiff systems encountered in diverse scientific and engineering domains.

The inspiration behind this research is to develop a super-implicit scheme following Cash's concept in [8] by introducing additional super future points to the existing fixed point formulae previously established by [7]. In subsequent sections, we will present the formulation, order of accuracy, stability analysis, convergence, and implementation of our proposed method.

2 | Formulation of the Method

In this section, a k-step super class of EBDf schemes is derived by throwing in an additional future point to the fixed point method by [7] to come up with a new super implicit method of the form:

$$\sum_{j=0}^k \alpha_j y_{n+j} = h\beta_k(f_{n+k} - \rho f_{n+k-1}) + h\beta_{k+1}f_{n+k+1}. \quad (5)$$

These techniques present fully implicit higher-order non-block schemes designed to approximate a single solution value at constant step size. The detailed derivation of the k-step super class of EBDf with step number two is presented, and the same procedure is employed to derive the differential coefficients of Taylor's series expansion for the remaining higher-order numerical schemes. Thus, the step number k is selected to lie within the interval $1 \leq k \leq 8$, in accordance with the approach outlined in [8].

Definition 1. The two-step Superclass of non-block Extended Backward Differentiation Formula (SEBDF2) is defined by

$$\sum_{j=0}^k \alpha_j y_{n+j} = h\beta_k(f_{n+k} - \rho f_{n+k-1}) + h\beta_{k+1}f_{n+k+1}, k = 2. \quad (6)$$

Definition 2. The linear operator L_i associated with SEBDF2 is defined as

$$L_2[y(x_n, h)]: \alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} - h\beta_2 f_{n+2} + h\rho\beta_2 f_{n+1} - h\beta_3 f_{n+3} = 0. \quad (7)$$

Expanding the associated approximate relationship for Eq. (7) as Taylor's series about any point x_n and collecting the like terms gives:

$$c_0 y(x_n) + c_1 h y'(x_n) + c_2 h^2 y''(x_n) + c_3 h^3 y'''(x_n) + \dots = 0, \quad (8)$$

where

$$\left. \begin{aligned} c_0 &= \alpha_0 + \alpha_1 + \alpha_2 = 0 \\ c_1 &= \alpha_1 + 2\alpha_2 - \beta_2(1 - \rho) - \beta_3 = 0 \\ c_2 &= \frac{1}{2}\alpha_1 + 2\alpha_2 - \beta_2(2 - \rho) - 3\beta_3 = 0 \\ c_3 &= \frac{1}{6}\alpha_1 + \frac{4}{3}\alpha_2 - \beta_2\left(2 - \frac{1}{2}\rho\right) - \frac{9}{2}\beta_3 = 0 \end{aligned} \right\}. \quad (9)$$

By normalizing the coefficient of y_{n+2} to one, Eq. (9) becomes:

$$\left. \begin{aligned} c_0 &= \alpha_0 + 1 + \alpha_2 = 0 \\ c_1 &= \alpha_1 + 2 - \beta_2(1 - \rho) - \beta_3 = 0 \\ c_2 &= \frac{1}{2}\alpha_1 + 2 - \beta_2(2 - \rho) - 3\beta_3 = 0 \\ c_3 &= \frac{1}{6}\alpha_1 + \frac{4}{3} - \beta_2\left(2 - \frac{1}{2}\rho\right) - \frac{9}{2}\beta_3 = 0 \end{aligned} \right\}. \quad (10)$$

Solving the set of Eq. (10), we obtain the following values of α_0 , α_1 , α_2 , β_2 and β_3 as in the table below:

Table 1. Coefficients of SEBDF2 scheme.

α_0	α_1	α_2	β_2	β_3
$\frac{8\rho + 5}{16\rho - 23}$	$\frac{4(2\rho - 7)}{16\rho - 23}$	1	$\frac{22}{16\rho - 23}$	$\frac{2(\rho + 2)}{16\rho - 23}$

Substituting these values in Eq. (7), the linear difference operator of the method in Eq. (5) becomes:

$$y_{n+2} = \frac{8\rho+5}{16\rho-23}y_n + \frac{4(2\rho-7)}{16\rho-23}y_{n+1} - \frac{22}{16\rho-23}hf_{n+2} + \frac{22}{16\rho-23}h\rho f_{n+1} + \frac{2(\rho+2)}{16\rho-23}hf_{n+3}. \quad (11)$$

Thus, the formula in Eq. (11) is termed a two-step Superclass of non-block Extended Backward Differentiation Formula (SEBDF2). It should be noted that the same procedure is applied for the derivation of the coefficients of the remaining k-step SEBDF schemes as follows:

For k = 1:

$$\alpha_0 = -1, \alpha_1 = 1, \beta_1 = -\frac{3}{2(2\rho-1)}, \beta_2 = \frac{1}{2} \frac{\rho+1}{2\rho-1}.$$

For k = 3:

$$\alpha_0 = \frac{14\rho+17}{76\rho-197}, \alpha_1 = -\frac{9(12\rho+11)}{76\rho-197}, \alpha_2 = \frac{9(2\rho+31)}{76\rho-197}, \alpha_3 = 1, \beta_2 = -\frac{150}{76\rho-197}, \beta_3 = \frac{6(\rho+3)}{76\rho-197}.$$

For k = 4:

$$\alpha_0 = -\frac{62\rho+111}{642\rho-2501}, \alpha_1 = \frac{8(57\rho+91)}{642\rho-2501}, \alpha_2 = -\frac{36(49\rho+59)}{642\rho-2501}, \alpha_3 = \frac{8(91\rho+501)}{642\rho-2501}, \alpha_4 = 1, \beta_3 = -\frac{1644}{642\rho-2501}, \beta_4 = \frac{36(\rho+4)}{642\rho-2501}.$$

For k = 5:

$$\alpha_0 = \frac{1}{3} \frac{167\rho+394}{936\rho-4973}, \alpha_1 = -\frac{5(88\rho+195)}{936\rho-4973}, \alpha_2 = \frac{20(81\rho+160)}{936\rho-4973}, \alpha_3 = -\frac{20}{3} \frac{628\rho+935}{936\rho-4973}, \alpha_4 = \frac{5(403\rho+1770)}{936\rho-4973}, \alpha_5 = 1, \beta_4 = -\frac{2940}{936\rho-4973}, \beta_5 = \frac{40(\rho+5)}{936\rho-4973}.$$

For k = 6:

$$\alpha_0 = -\frac{2(118\rho+345)}{5860\rho-39981}, \alpha_1 = \frac{1}{3} \frac{6145\rho+17268}{5860\rho-39981}, \alpha_2 = -\frac{225(36\rho+95)}{5860\rho-39981}, \alpha_3 = \frac{100(199\rho+468)}{5860\rho-39981}, \alpha_4 = -\frac{50}{3} \frac{2318\rho+4107}{5860\rho-39981}, \alpha_5 = \frac{9(2129\rho+8660)}{5860\rho-39981}, \alpha_6 = 1, \beta_5 = -\frac{21780}{5860\rho-39981}, \beta_6 = \frac{200(\rho+6)}{5860\rho-39981}.$$

For k = 7:

$$\alpha_0 = \frac{5}{3} \frac{433\rho+1509}{24840\rho-208903}, \alpha_1 = -\frac{14}{3} \frac{1476\rho+5005}{24840\rho-208903}, \alpha_2 = \frac{7}{3} \frac{12815\rho+41762}{24840\rho-208903}, \alpha_3 = -\frac{175}{3} \frac{1352\rho+4137}{24840\rho-208903}, \alpha_4 = \frac{175}{3} \frac{2493\rho+6797}{5860\rho-39981}, \alpha_5 = -\frac{70}{3} \frac{9692\rho+19901}{24840\rho-208903}, \alpha_6 = \frac{7(15859\rho+63070)}{24840\rho-208903}, \alpha_7 = 1, \beta_6 = -\frac{106540}{24840\rho-208903}, \beta_7 = \frac{700(\rho+7)}{24840\rho-208903}.$$

For k = 8:

$$\alpha_0 = -\frac{5(1802\rho+7287)}{410830\rho-4134649}, \alpha_1 = \frac{10}{3} \frac{28259\rho+112008}{410830\rho-4134649}, \alpha_2 = -\frac{392}{3} \frac{3441\rho+13270}{410830\rho-4134649}, \alpha_3 = \frac{98}{3} \frac{39845\rho+147664}{410830\rho-4134649}, \alpha_4 = -\frac{4900}{3} \frac{1577\rho+5487}{410830\rho-4134649}, \alpha_5 = \frac{490}{3} \frac{23277\rho+72152}{410830\rho-4134649}, \alpha_6 = -\frac{1960}{3} \frac{7549\rho+17618}{410830\rho-4134649}, \alpha_7 = \frac{2(1178937\rho+4697840)}{410830\rho-4134649}, \alpha_8 = 1, \beta_8 = -\frac{1996120}{410830\rho-4134649}, \beta_9 = \frac{9800(\rho+8)}{410830\rho-4134649}.$$

To guarantee the absolute and 0-stability of the SEBDF2 scheme, the free parameter ρ is constrained within the interval $-1 \leq \rho < 1$, as previously established in [6], [9–11]. By varying ρ , diverse sets of super implicit A-stable and $A(\alpha)$ -stable higher-order schemes are generated.

Notably, when $\rho = 0$, the SEBDF schemes reduce to Cash's k-step EBDP schemes in [8]. Thus, our proposed numerical algorithms encompass EBDP methods as a subclass. For numerical implementation and computation of the SEBDF2 algorithm, *Eq. (11)* is modified by substituting $\rho = \frac{1}{5}$ to obtain:

$$y_{n+1} = -\frac{1}{3}y_{n-1} + \frac{4}{4}y_n + \frac{10}{9}hf_{n+1} - \frac{2}{9}hpf_n - \frac{2}{9}hf_{n+2}. \quad (12)$$

3 | Order of Accuracy and Error Constant of SEBDF2

To investigate the order and error constant of *Eq. (11)*, we begin with the introduction of the following definition:

Definition 3 (order). The linear difference operator *Eq. (7)* and its associated numerical method *Eq. (6)* are said to be of order p , if in *Eq. (8)*,

$$C_0 = C_1 = C_2 = \dots = C_p = 0 \text{ and } C_{p+1} \neq 0, \quad (12)$$

where C_{p+1} is called an error constant [12].

Therefore, the order and error constant of the method are presented by substituting the values of α_j and β_j in *Eq. (9)* to obtain:

$$\left. \begin{aligned} C_0 &= -\frac{8\rho+5}{16\rho-23} - \frac{4(2\rho-7)}{16\rho-23} + 1 = 0 \\ C_1 &= -\frac{4(2\rho-7)}{16\rho-23} + 2 - (1-\rho)\left(-\frac{22}{16\rho-23}\right) - \frac{2(\rho+2)}{16\rho-23} = 0 \\ C_2 &= \frac{1}{2}\left(-\frac{4(2\rho-7)}{16\rho-23}\right) + 2 - (2-\rho)\left(-\frac{22}{16\rho-23}\right) - 3\left(\frac{2(\rho+2)}{16\rho-23}\right) = 0 \\ C_3 &= \frac{1}{6}\left(-\frac{4(2\rho-7)}{16\rho-23}\right) + \frac{4}{3} - \left(2 - \frac{1}{2}\rho\right)\left(-\frac{22}{16\rho-23}\right) - \frac{9}{2}\left(\frac{2(\rho+2)}{16\rho-23}\right) = 0 \\ C_4 &= \frac{1}{24}\left(-\frac{4(2\rho-7)}{16\rho-23}\right) + \frac{2}{3} - \left(\frac{4}{3} - \frac{1}{6}\rho\right)\left(-\frac{22}{16\rho-23}\right) - \frac{9}{2}\left(\frac{2(\rho+2)}{16\rho-23}\right) = 0 \end{aligned} \right\}. \quad (13)$$

The formulae in *Eq. (13)* are simplified and expressed as

$$\left. \begin{aligned} C_0 &= 0 \\ C_1 &= 0 \\ C_2 &= 0 \\ C_3 &= 0 \\ C_4 &= -\frac{1}{6} \frac{14\rho+17}{16\rho-23} \neq 0 \end{aligned} \right\}. \quad (14)$$

Hence, in accordance with *Definition 3*, we conclude that the SEBDF2 method is of order three with the error constant given as

$$C_4 = -\frac{1}{6} \frac{14\rho+17}{16\rho-23} \neq 0, \quad (15)$$

The Local Truncation Error (LTE) of SEBDF2 is given by

$$\pm \frac{1}{6} \frac{14\rho+17}{16\rho-23} h^4 y^{(4)}(x_n) + \dots \quad (16)$$

Table 2 below provides a comprehensive overview of the error constants and orders associated with the stiffly-accurate implicit Superclass of Extended Backward Differentiation Formula (SEBDF) schemes for the range of $1 \leq k \leq 8$, where k represents the step number of the method.

Each row in the table corresponds to a specific SEBDF scheme, denoted as SEBDF1 through SEBDF8. The error constants column indicates the numerical value associated with the error constant for each scheme, and the order of the method column signifies the order of accuracy for the respective SEBDF scheme.

Table 2. The orders and error constants of the SEBDF schemes for $1 \leq k \leq 8$.

Method	Error Constant	Order
SEBDF1	$c_3 = -\frac{1}{12} \frac{8\rho+5}{2\rho-1}$	2
SEBDF2	$c_4 = -\frac{1}{6} \frac{14\rho+17}{16\rho-23}$	3
SEBDF3	$c_5 = -\frac{1}{10} \frac{62\rho+111}{76\rho-197}$	4
SEBDF4	$c_6 = -\frac{1}{5} \frac{167\rho+394}{642\rho-2501}$	5
SEBDF5	$c_7 = \frac{2}{483} \frac{79666\rho-23805}{936\rho-4973}$	6
SEBDF6	$c_8 = -\frac{5}{14} \frac{433\rho+1509}{5860\rho-39981}$	7
SEBDF7	$c_9 = -\frac{5}{18} \frac{1802\rho+7287}{24840\rho-208903}$	8
SEBDF8	$c_{10} = -\frac{7}{9} \frac{8389\rho+38596}{410830\rho-4134649}$	9

4 | Stability Analysis

The stability region of a numerical integration method is a region in the complex plane where the numerical solution remains bounded for a certain class of problems. The stability region is crucial for understanding the behavior of numerical methods, especially for solving ODEs or Partial Differential Equations (PDEs).

Typically, the stability regions are illustrated in the complex plane, and they indicate the regions where the numerical solution does not exhibit unbounded growth or oscillations. The shape and size of the stability region are influenced by the properties of the numerical method, such as its order and stability characteristics [13].

Absolute stability regions and zero-stable SEBDF schemes are presented in this section. To investigate zero and A-stability of SEBDF2, we put the scalar test first order ODE of the form $y' = \lambda y$, where λ is a complex constant with negative real parts in Eq. (11), we obtain:

$$y_{n+2} = \frac{8\rho+5}{16\rho-23}y_n + \frac{4(2\rho-7)}{16\rho-23}y_{n+1} - \frac{22}{16\rho-23}h\lambda y_{n+2} + \frac{22}{16\rho-23}h\lambda \rho y_{n+1} + \frac{2(\rho+2)}{16\rho-23}h\lambda y_{n+3}. \quad (17)$$

Let $\bar{h} = h\lambda$ and assume a solution of the form $y_n = t^n$ in Eq. (17). This leads to a stability polynomial given as

$$t^2 = \frac{8\rho+5}{16\rho-23} + \frac{4(2\rho-7)}{16\rho-23}t - \frac{22}{16\rho-23}\bar{h}t^2 + \frac{22}{16\rho-23}\bar{h}\rho t + \frac{2(\rho+2)}{16\rho-23}\bar{h}t^3. \quad (18)$$

Putting $\bar{h} = h\lambda = 0$, in Eq. (18) leads to the first characteristics polynomial as

$$t^2 - \frac{8\rho+5}{16\rho-23} - \frac{4(2\rho-7)}{16\rho-23}t = 0. \quad (19)$$

Solving Eq. (19) for t , we obtain the following roots:

$$t = 1, t = -\frac{8\rho+5}{16\rho-23}. \quad (20)$$

Definition 4 (root condition). A polynomial of a LMM is said to satisfy the root condition if all its roots lie within or on the unit circle, with those on the boundary being simple. In other words, all roots satisfy $|t| \leq 1$ and any that satisfy $|t| = 1$ are simple [14].

Definition 5 (zero-stability). A LMM is said to be zero stable if its first characteristic polynomial $\pi(t)$ satisfies the root condition [14].

By *Definition 5*, the SEBDF2 scheme is zero stable for any suitable value of ρ within the interval $-1 \leq \rho < 1$. To verify the suitability of ρ , we randomly selected five values within the aforementioned interval for testing zero stability, as shown table below.

Table 3. Roots for different values of ρ .

ρ	$ t $	$ t \leq 1$	Stability
-1	$t = 0.07692, t = 1$	Satisfied	Zero stable
0.5	$t = 0.60000, t = 1$	Satisfied	Zero stable
0.2	$t = 0.30000, t = 1$	Satisfied	Zero stable
-0.875	$t = 0.05405, t = 1$	Satisfied	Zero stable
-0.75	$t = 0.02857, t = 1$	Satisfied	Zero stable

Hence, the SEBDF2 method exhibits zero stability for most values of ρ , except for $\rho = 1$, where it becomes zero-unstable due to roots exceeding the stability threshold.

Definition 6 (A-stability). A LMM is said to be A-stable if the absolute value of the root (s) of the stability polynomial of the numerical integrator lies in the open left half of the complex plane of the stability region [15].

Definition 7 ($A(\alpha)$ -stability). A numerical method is said to be $A(\alpha)$ -stable for some $\alpha[0, \infty]$ if the wedge $S_\alpha = \{z: |\text{Arg}(-z)| < \alpha, z \neq 0\}$ is contained in its region of absolute stability [15].

Therefore, the boundary of the stability region of the SEBDF2 method is determined by substituting the set of points $t = e^{i\theta}$, $0 \leq \theta \leq 2\pi$ in *Eq. (18)*. The graphs of the stability region of the method are plotted in the Maple18 environment and are shown in the figures below:

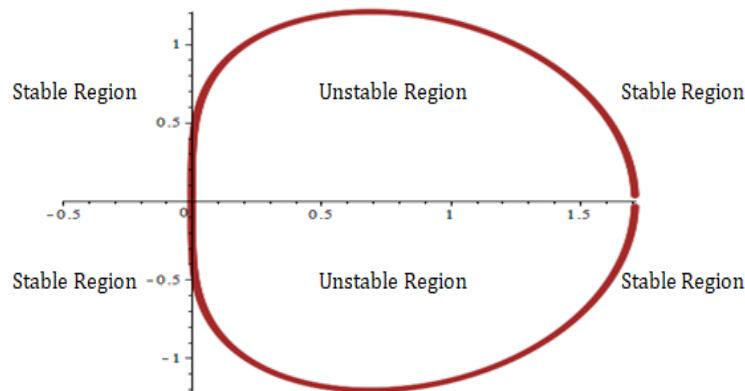


Fig. 1. The stability region of SEBDF2 when $\rho = 0.2$.

Thus, *Eq. (11)* exhibits absolute stability across the entire left half plane, signifying its A-stability for ρ value of 0.2. this A-stability makes the method well-suited for effective numerical integration of stiff IVPs.

Figs. 2 and 3 depict the combined absolute stability region plots for SEBDF schemes with step numbers ranging from 1 to 4.

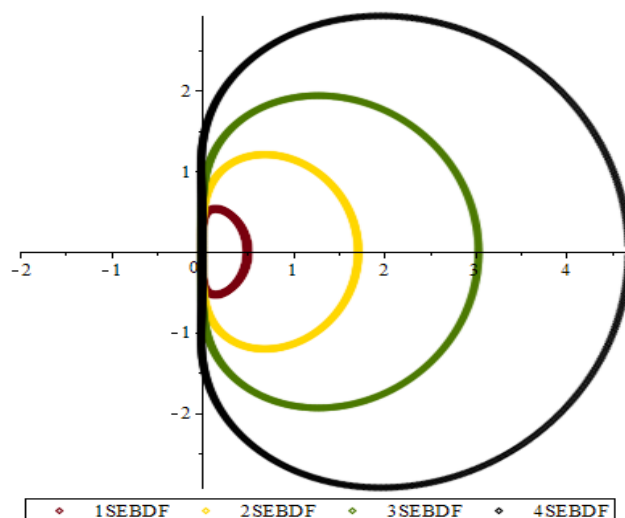


Fig 2. Stability regions for SEBDF schemes when $\rho = 0.2$.

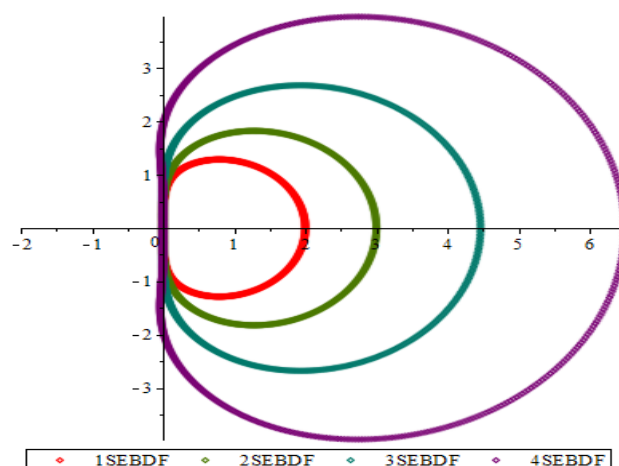


Fig. 3. Stability regions for SEBDF schemes when $\rho = -0.25$.

These figures showed that the SEBDF schemes for $1 \leq k \leq 4$ are all A-stable since the stability regions cover the whole left half complex plane.

Similarly, the $A(\alpha)$ -stability regions for the remaining SEBDF schemes ranging from 5 to 8 are shown in the figures below.

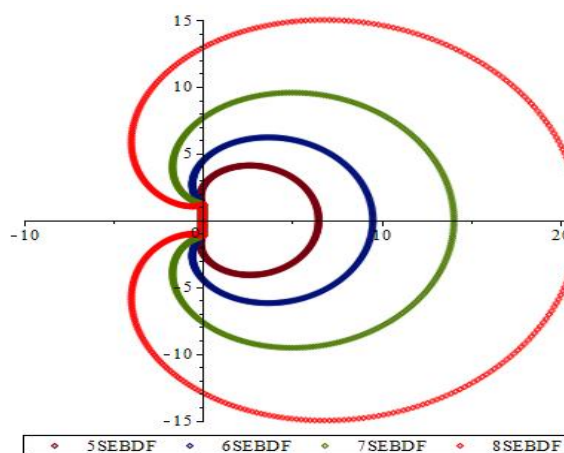


Fig. 4. Stability regions for SEBDF schemes when $\rho = 0.333$.

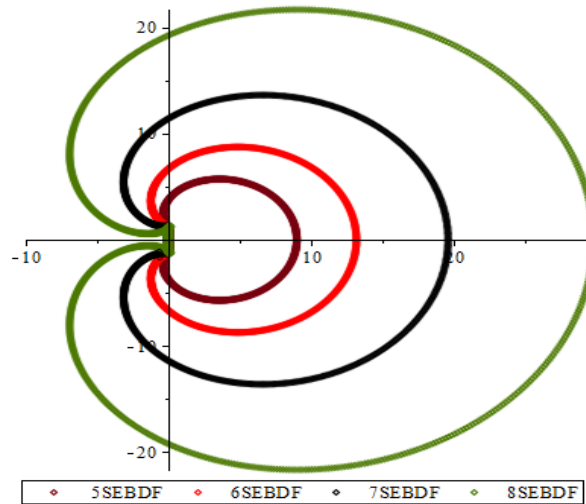


Fig. 5. Stability regions for SEBDF schemes when $\rho = -0.2$.

Based on Figs. 4 and 5, the SEBDF schemes ranging from 5 to 8 possess the region of absolute stability, which contains almost the whole of the left half complex plane. Hence, we conclude that the schemes are $A(\alpha)$ -stable and are suitable for solving stiff systems of IVPs.

5 | Convergence of SEBDF2 Method

Convergence is a fundamental property that every valid LMM must possess. In this section, we explore the convergence of the method based on Dahlquist's equivalence theorem presented in [12]. Lambert [12] emphasizes that both consistency and zero stability are indispensable prerequisites for the convergence of any numerical method. Thus, consistency influences the magnitude of LTE, while zero stability determines how the error propagates at each calculation step.

Convergence further signifies that the approximate solutions produced by the developed methods tend to approach the theoretical solution as the step size becomes infinitesimally small. In essence, the convergence property ensures that the numerical method becomes more accurate as the step size decreases [15].

Any method that lacks either consistency or zero stability is deemed non-convergent and, as a result, is unsuitable for practical applications in solving differential equations. Therefore, convergence is a crucial criterion for determining the suitability of the numerical method for solving real-world problems.

Definition 8 (consistency). An LMM is said to be consistent if it has an order p greater than or equal to 1. It follows that an LMM is consistent if

- I. $\pi(1) = 0$,
- II. $\pi'(1) = \sigma(1)$.

where π and σ denote the first and second characteristics polynomial of an LMM [12].

Theorem 1 (Dahlquist equivalence theorem). The necessary and sufficient conditions for an LMM to be convergent are that it is consistent and zero-stable [12].

Theorem 2. The SEBDF2 scheme is convergent.

Proof: to establish the convergence of the SEBDF2 method, it is adequate to demonstrate that the method satisfies both consistency and zero stability criteria. We will begin by demonstrating that the SEBDF2 method is consistent.

Let the first and second characteristics polynomial of Eq. (11) be defined as

$$\pi(r) = r^2 - \frac{4(2\rho-7)}{16\rho-23}r - \frac{8\rho+5}{16\rho-23}, \quad \sigma(r) = \frac{2(\rho+2)}{16\rho-23}r^3 - \frac{22}{16\rho-23}r^2 + \frac{22\rho}{16\rho-23}r \quad \text{and} \quad \pi'(r) = 2r - \frac{4(2\rho-7)}{16\rho-23}.$$

It follows from the *Definition 8* that:

$$\pi(1) = 1 - \frac{4(2\rho-7)}{16\rho-23} - \frac{8\rho+5}{16\rho-23} = 0. \quad (21)$$

Hence, the first condition in (I) is satisfied.

$$\begin{aligned} \pi'(1) &= 2 - \frac{4(2\rho-7)}{16\rho-23} = \frac{6(4\rho-3)}{16\rho-23}, \\ \sigma(1) &= \frac{2(\rho+2)}{16\rho-23} - \frac{22}{16\rho-23} + \frac{22\rho}{16\rho-23} = \frac{6(4\rho-3)}{16\rho-23}, \\ \Rightarrow \pi'(1) &= \frac{6(4\rho-3)}{16\rho-23} = \sigma(1). \end{aligned} \quad (22)$$

Therefore, the second condition is also satisfied.

It has thus shown that consistency conditions are therefore met. Hence, the SEBDF2 method is consistent. In accordance with *Theorem 1*, we conclude that the SEBDF2 method converges since the two conditions of consistency and zero stability are satisfied.

5 | Implementation of SEBDF2 Method

In this section, we only consider the implementation of the SEBDF2 method. Newton's iteration is applied for the implementation of the method. The description of the iteration is given below; we first start by defining the error.

Definition 9 (absolute error). Let y_i and $y(x_i)$ be the exact and approximate solutions of the given first order ODE *Eq. (1)*. Then the absolute error is given by

$$(\text{error}_i)_t = |(y_i)_t - (y(x_i))_t|. \quad (23)$$

Let T be the total number of steps and N be the number of equations. Then, the maximum absolute error is defined as

$$\text{MAXE} = \max_{1 \leq i \leq T} (\max_{1 \leq i \leq N} (\text{error}_i)_t). \quad (24)$$

Let

$$F = y_{n+2} - \frac{8\rho+5}{16\rho-23}y_n - \frac{4(2\rho-7)}{16\rho-23}y_{n+1} + \frac{22}{16\rho-23}hf_{n+2} - \frac{22}{16\rho-23}h\rho f_{n+1} - \frac{2(\rho+2)}{16\rho-23}hf_{n+3}. \quad (25)$$

In order to rewrite *Eq. (25)* in standard form, we replace n by $n-1$ to obtain:

$$F = y_{n+1} - \frac{8\rho+5}{16\rho-23}y_{n-1} - \frac{4(2\rho-7)}{16\rho-23}y_n + \frac{22}{16\rho-23}hf_{n+1} - \frac{22}{16\rho-23}h\rho f_n - \frac{2(\rho+2)}{16\rho-23}hf_{n+2}. \quad (26)$$

This implies that

$$F = y_{n+1} + \frac{22}{16\rho-23}hf_{n+1} - \frac{22}{16\rho-23}h\rho f_n - \frac{2(\rho+2)}{16\rho-23}hf_{n+2} - \varepsilon, \quad (27)$$

where, $\varepsilon = \frac{8\rho+5}{16\rho-23}y_{n-1} + \frac{4(2\rho-7)}{16\rho-23}y_n$ is the back value.

Let $y_{n+1}^{(i+1)}$ denote the $(i+1)^{\text{th}}$ iterative values of y_{n+1} and define

$$e_{n+1}^{(i+1)} = y_{n+1}^{(i+1)} - y_{n+1}^{(i)}. \quad (28)$$

Newton's iteration for SEBDF2 takes the form

$$y_{n+1}^{(i+1)} = y_{n+1}^{(i)} - \left(F'_1(y_{n+1}^{(i)})\right)^{-1} \left(F_1(y_{n+1}^{(i)})\right). \quad (29)$$

This is also written as

$$\left(F'_1(y_{n+1}^{(i)})\right) e_{n+1}^{(i+1)} = -\left(F_1(y_{n+1}^{(i)})\right). \quad (30)$$

Eq. (30) is equivalent to the following form:

$$\left(1 + \frac{22}{16\rho-23} h \frac{\partial f_{n+1}}{\partial y_{n+1}}\right) e_{n+1}^{(i+1)} = -\left(y_{n+1} - \frac{22}{16\rho-23} h f_{n+1} + \frac{22}{16\rho-23} h \rho f_n + \frac{2(\rho+2)}{16\rho-23} h f_{n+2} + \varepsilon\right). \quad (31)$$

The computer code in C programming language is written for the implementation of Eq. (31).

6 | Test Problems and Numerical Results

To validate the performance of the SEBDF2 method, the following systems of first-order stiff IVPs are tested:

Problem 1. Consider the stiff Initial Value Problem (IVP) taken from [12]:

$$y'_1 = -21y_1 + 19y_2 - 20y_3, \quad y_1(0) = 1, \quad 0 \leq x \leq 10,$$

$$y'_2 = 19y_1 - 21y_2 + 20y_3, \quad y_2(0) = 0,$$

$$y'_3 = 40y_1 - 40y_2 - 40y_3, \quad y_3(0) = -1.$$

The theoretical solution is given by

$$y_1(x) = 0.5(e^{-2x} + e^{-40x}(\cos(40x) + \sin(40x))),$$

$$y_2(x) = 0.5(e^{-2x} - e^{-40x}(\cos(40x) + \sin(40x))),$$

$$y_3(x) = 2e^{-40x} \left(-\frac{1}{2} \cos(40x) + \frac{1}{2} \sin(40x)\right),$$

where the eigenvalues of the given system are -2 , $-40 + 40i$ and $-40 - 40i$.

Problem 2. This stiff problem is taken from [16]:

$$y'_1 = 9y_1 + 24y_2 + 5 \cos(x) - \frac{1}{3} \sin(x), \quad y_1(0) = \frac{4}{3}, \quad 0 \leq x \leq 10,$$

$$y'_2 = -24y_1 - 51y_2 - 9 \cos(x) + \frac{1}{3} \sin(x), \quad y_2(0) = \frac{2}{3},$$

whose eigenvalues are given by -3 , and -39 and its exact solution is given by

$$y_1(x) = 2e^{-3x} - e^{-39x} + \frac{1}{3} \cos(x),$$

$$y_2(x) = -e^{-3x} + 2e^{-39x} - \frac{1}{3} \cos(x).$$

Problem 3. Consider the stiff Initial Value Problem (IVP) taken from [17]

$$y'_1 = -0.1y_1 - 49.9y_2, y_1(0) = 2, 0 \leq x \leq 10,$$

$$y'_2 = -50y_2, y_2(0) = 1,$$

$$y'_3 = 70y_2 - 120y_3, y_3(0) = 2.$$

The theoretical solution is given by

$$y_1(x) = e^{-0.1x} + e^{-50x},$$

$$y_2(x) = e^{-50x},$$

$$y_3(x) = e^{-50x} + e^{-120x}.$$

where the eigenvalues of the system are -0.1 , -120 and -50 .

The numerical results for the test problems are tabulated. The problems are solved using the SEBDF2 method, two-step Backward Differentiation Formula (BDF2) and two-step fixed point Superclass of Backward Differentiation Formula (SBDF2). Additionally, for convenient cross-referencing, the BDF2 from [5] is provided as

$$y_{n+2} = -\frac{1}{3}y_n + \frac{4}{3}y_{n+1} + \frac{2}{3}hf_{n+2}. \quad (32)$$

Similarly, the SBDF2, as proposed in [7], is expressed as

$$y_{n+2} = -\frac{1}{31}y_n + \frac{32}{31}y_{n+1} + \frac{16}{31}hf_{n+2} + \frac{14}{31}hf_{n+1}. \quad (33)$$

Therefore, the SEBDF2 in Eq. (12) takes the following standard form:

$$y_{n+2} = -\frac{1}{3}y_n + \frac{4}{4}y_{n+1} + \frac{10}{9}hf_{n+2} - \frac{2}{9}hpf_{n+1} - \frac{2}{9}hf_{n+3}. \quad (34)$$

The maximum error and computation time for different methods are presented and compared in the tables below. The notations used in the tables are:

H: step size.

METHOD: methods used to solve the problems.

TS: total number of integration steps.

MAXE: maximum error.

CPU TIME: computation time in seconds.

Table 4. Numerical results for Problem 1.

H	Method	Maxe	Cpu Time
10^{-2}	BDF2	2.62644E-001	2.43100E-003
	SBDF2	1.50594E-001	2.74800E-003
	SEBDF2	1.09829E-001	1.59200E-004
10^{-4}	BDF2	4.09407E-003	2.47600E-002
	SBDF2	2.18868E-003	4.70600E-002
	SEBDF2	7.28330E-004	2.62400E-003
10^{-6}	BDF2	4.11250E-005	4.61300E+001
	SBDF2	2.19339E-005	4.83400E+001
	SEBDF2	7.26022E-006	4.53300E-001

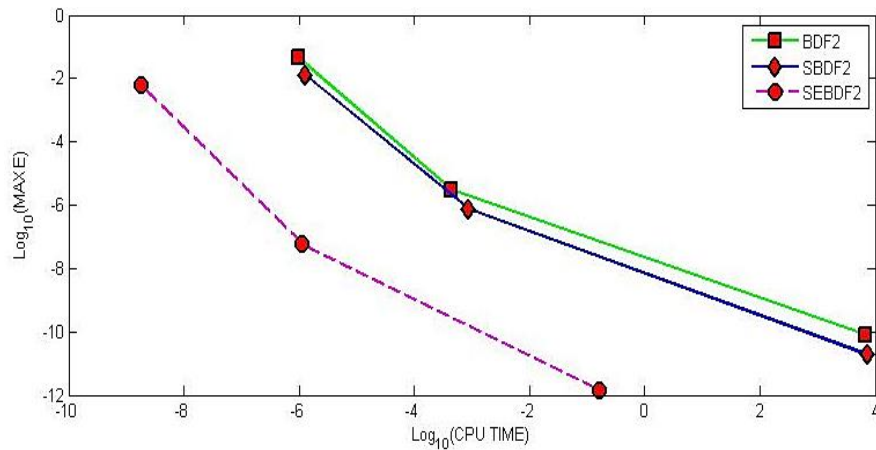
Table 5. Numerical results for Problem 2.

H	Method	Maxe	CPU Time
10^{-2}	BDF2	1.35436E-001	1.36400E-002
	SBDF2	1.15523E-001	2.10200E-002
	SEBDF2	6.84772E-002	2.35200E-003
10^{-4}	BDF2	2.83293E-003	2.24100E-001
	SBDF2	1.51515E-003	2.76300E-001
	SEBDF2	6.97801E-004	3.18400E-002
10^{-6}	BDF2	2.84863E-005	2.81400E+001
	SBDF2	1.51931E-005	3.24800E+001
	SEBDF2	6.96632E-006	4.60200E-001

Table 6. Numerical results for Problem 3.

H	Method	Maxe	Cpu Time
10^{-2}	BDF2	9.43984E-002	2.47100E-004
	SBDF2	7.30662E-002	2.74200E-004
	SEBDF2	7.28373E-002	3.13100E-005
10^{-4}	BDF2	5.76665E-003	2.58900E-002
	SBDF2	3.09897E-003	2.65300E-002
	SEBDF2	9.21629E-004	3.15400E-003
10^{-6}	BDF2	5.85376E-005	3.60900E-001
	SBDF2	3.12224E-005	4.91000E-001
	SEBDF2	9.19728E-006	2.31600E-002

The results presented in *Tables 4* and *5* highlight the superior accuracy of the SEBDF2 scheme compared to BDF2 and SBDF2 methods. However, when considering computation time, our novel method performs slightly better than BDF2 and SBDF2 schemes. The performance and efficiency of our algorithm arise from the incorporation of the super future point in our formulations. To visually illustrate the performance of our method in comparison to the existing BDF2 and SBDF2 methods, the efficiency curves have been generated. These curves dict $\log_{10}(\text{MAXE})$ plotted against $\log_{10}(\text{CPU TIME})$ for each tested problem. The graphs are presented, organized in a sequential manner below, offering a clear representation of the scaled maximum error across varying step sizes in a Matlab environment.

**Fig. 6. Efficiency curves for Problem 1.**

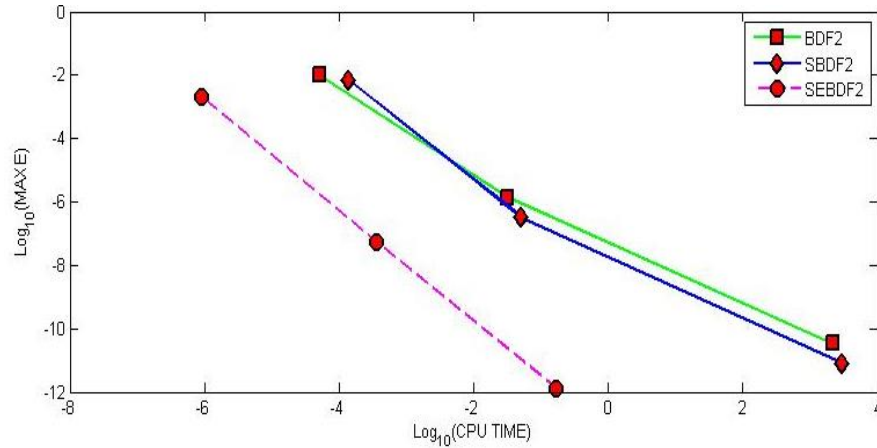


Fig. 7. Efficiency curves for Problem 2.

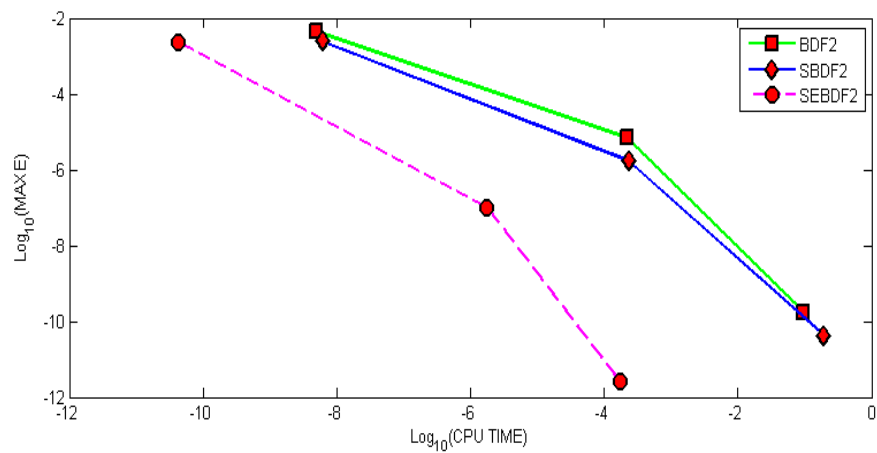


Fig. 8. Efficiency curves for Problem 3.

7 | Discussion

The efficiency curves plotted for each problem provide valuable insights into the comparative performance of the existing BDF2, SBDF2 and our proposed SEBDF2 numerical method. The logarithmic scaling of both the Maximum Error (MAXE) and the Computation Time (CPU TIME) allows for a clearer assessment of accuracy and convergence behavior.

Upon examination of the efficiency curves, it is evident that our novel SEBDF2 method exhibits superior accuracy compared to both BDF2 and SBDF2 schemes. The lower values of MAXE indicate that our method achieves more accurate results across varying step sizes (H).

However, the efficiency curves also show that the CPU TIME of our method is more than that of BDF2 and SBDF2, as reflected in the tables. This suggests that while SEBDF2 enhances accuracy, it does so without significantly sacrificing computational efficiency.

The decision to incorporate a super future point into our method appears to be justified, as it contributes to improved accuracy and computation time observed in the efficiency curves. This visual representation reinforces the earlier findings from the tabulated results, emphasizing the overall effectiveness of SEBDF2 in balancing accuracy and computational efficiency.

8 | Conclusion

In conclusion, this paper introduces an implicit superclass of non-block extended BDF designed for the numerical integration of stiff IVPs. The presented SEBDF methods exhibit optimal stability properties, with established necessary and sufficient conditions for convergence. Through a thorough analysis of stability and convergence, the study demonstrates that the proposed numerical integration schemes are consistent, zero stable and convergent.

Furthermore, the absolute stability regions of the SEBDF methods highlight their A-stability of order up to 5 and $A(\alpha)$ -stability of order up to 9, emphasizing their robustness in handling stiff IVPs. The implementation of the SEBDF2 method employs Newton iteration, and the numerical results obtained from solving some selected stiff IVPs showcase the superiority of the proposed approach over existing BDF2 and SBDF2 schemes.

In essence, the research contributes valuable advancements to the field of numerical integration, particularly in addressing the challenges posed by stiff systems of IVPs. The demonstrated effectiveness and improved performance of the proposed SEBDF2 method underscore its potential as a reliable tool for numerically solving stiff IVPs, offering enhanced accuracy and stability compared to existing methods.

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Author Contribution

Conceptualization, H.M. and B.A.; Methodology, H.M. and B.A.; Software, H.M.; Validation, H.M. and B.A.; Formal analysis, H.M.; Investigation, B.A.; Resources, H.M.; Data maintenance, B.A.; Writing-creating the initial design, H.M.; Writing-reviewing and editing, H.M. and B.A.; Visualization, B.A.; Monitoring, H.M.; Project management, H.M.; Funding procurement, U.M.Y.U. and A.U.K. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors affirm that they have no conflicts of interest related to the publication of this paper.

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